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SCATTERING OF FREE ELECTRONS WITH HYDROGEN ATOMS IN PROTON EXCHANGE MEMBRANE FUEL CELL

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Abstract

This study examines the evolution of the Klein-Nishina (KN) cross section for hydrogen and platinum atoms in relativistic and non-relativistic scenarios. Using online MATLAB tools, the constructed model of KN cross section for both situations is calculated. The observation demonstrates that as electron energy increases, electronic and atomic KN cross section lowers, which lessens the relationship between the incoming electron and the target atom. The importance of atomic size is demonstrated by a comparison of the KN cross sections of hydrogen and platinum, with platinum possessing a higher cross section because of its greater size and more scattering centers. Higher atomic numbers result in greater interaction between sites and bigger cross sections, and they also play a role in this relationship. The variations in cross sections are also influenced by electron binding effects, especially in the instance of hydrogen. It is demonstrated that relativistic effects have a major impact on the KN cross section, including an exponential decline seen as the energy of electrons increases. In the relativistic domain, the electron's increased mass and decreased wavelength increase scattering probability and produce a greater cross section than in the non-relativistic case. This research sheds light on the variables affecting KN cross sections and their influence on radiation therapy, medical imaging, and materials science.

Keywords: KN cross section, Hydrogen, Platinum, relativistic and non-relativistic

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1. Introduction

In recent years, fuel cells made from hydrogen have drawn interest as a practical alternative energy source. Generally speaking, fuel cells use fuels like the gas hydrogen, methanol, or natural gas to transform the chemical energy contained in the fuel they contain into direct current (DC) without intermediary the combustion process, as is the case of traditional engines [1]. Fuel cells are a potential candidate for an environmentally friendly form of energy technology in the future due to their increased efficiency and low emissions. The fuel cells market and, consequently, the shift to a hydrogen economy are determined by the kind of fuel cell, the cost of the components, and the production processes. The price of fuel cells has dropped by 80% in the last couple of decades (since the 1990s), thanks to technological developments. Additionally, it is anticipated that the price of platinum will decline due to the rising demand for natural resources [2]. An fuel cell is an electrochemical machine that uses two redox processes to transform the chemical energy of a fuel (typically hydrogen) plus an oxidizing agent (commonly oxygen) into electrical energy [3]. Over the past three decades, as clean energy technologies are sought after globally for environmental and sustainable development goals, the proton exchange membrane fuel cell (PEMFC) has attracted a lot of interest. PEMFCs are devices which employ hydrogen fuel and transform chemical energies directly into electricity, bypassing the limitations of the Carnot cycle. As a result, they are more efficient and emit almost no emissions in comparison to conventional electricity-generating technologies and direct consuming of fossil fuels.

A single PEMFC is typically built in a hierarchical form, with a proton exchange membrane serving as the center layer through which primarily protons can pass. The catalyst layer (CL) of the anode and cathode, the gas diffusion layer (GDL) between the two electrodes, and the bipolar plates are arranged in order from the center to the edges. Together, the membrane, CLs, and GDLs are referred to as membrane electrode assemblies (MEA), and their physical makeup could be compared to that of porous media with multi-scale pores. Grooves called gas flow channels (GFCs) are mechanically carved into the innermost layer of the polar plate [4]. During cell operation, hydrogen and air are delivered into the cell via the flow channel and, in turn, pass through the anode's and cathode's respective gas diffusion layers to reach the catalyst layer. The molecules of hydrogen are depleted of their electrons and broken down into protons in the catalyst, which is the layer of the anode. To create an electric current, electrons are required to move through an external circuit. The formed electron, proton and residue goes interaction in effective area called, scattering cross sections. The scattering region can be calculated by using equation (1) from differential cross section phenomenon [5].

$$\frac{d\sigma}{d\Omega} = \frac{r_e^2}{2}\left(\frac{k'}{k_0}\right)^2 (1 + cos^2\theta) \qquad (1)$$

In terms of the wavelengths of the photons, Compton described this relationship as follows:

$$\lambda' - \lambda = 1 - cos\theta \qquad (2)$$

where λ and λ' are the photon's pre- and post-deflection Compton wavelengths [6].

In this work authors are applying Klein-Nishina (KN) cross section in the framework of electrode scattering which helpful insights about the connection among electrons and the electrode materials. In order to maximize the effectiveness and effectiveness of PEMFCs, it is essential to comprehend the KN cross section in this particular system. Electrochemical reactions in PEMFCs are greatly aided by electrode materials like platinum or other catalysts. As they engage with electrode surfaces during fuel cell operation, produced electrons experience scattering events. The likelihood of each of these scattering events occurring is measured using the KN cross section. The information regarding scattering in PEMFCs and its effects on performance can be examined by the KN cross section around an electrode scattering. On taking account the KN cross section in electrodes dispersion within PEMFCs offers useful knowledge for enhancing the design, functionality, and longevity of these energy-converting devices. It may direct the choice of materials and electrode engineering, and it can promote PEMFC technology for a variety of uses, such as transport and stationary power generation.

II. Literature Review

The initial gas-based voltaic cell powered by a mixture of hydrogen and oxygen was created by Sir William Grove in 1839, the same year he also put forth the notion of the fuel cell's effect. Ostwald laid the theoretical groundwork for fuel cell research in 1894. When attempting to understand the rate of electromechanical processes in fuel cells, Van Santen developed the Ostwald-proposed step rule concept [7]. In the 1920s, Lawaczek created numerous schemes for hydrogen-powered automobiles, trucks, buses, trains, and engines. He also made a substantial contribution to the development of pressurized electrolyzes. Although knowing that the idea for fuel cells first emerged in the beginning of the 1840s, it wasn't until Francis T. Bacon began researching them between 1932 and 1952 that this technology was once again developed, allowing the very first time the development and evaluation of a 5 kW hydrogen fuel cell stack. Later, this technology was created for the life support, guiding, and navigation systems used in NASA's Gemini and Apollo programs [8]. During the course of the last 20 years, the fuel cell sector has made enormous strides, leading to discussions about making investments in hydrogen. The development of fuel cell automobiles was a focus for several decades for automakers from various nations. The first commercially available fuel cell vehicle was released by Toyota in 2014, capping years of research and development work. As a result, the public began to view fuel cell cars as a significant component of the next generation of mobility rather than as an experimental technology. Countries including China, the US, Japan, and a number of European nations concentrated their efforts on advancing this technology throughout the course of the following five years [9].

From 2022 and 2027, the worldwide fuel cell industry is anticipated to increase from an USD 3 billion economy to a USD 9 billion economy at a 26.0% CAGR [10]. Over the course of the last few years, scientific research has also grown more interested in fuel cells. The peak growth in patent applications in the hydrogen-based fuel cell industry [11] (23% increase) from 2016 to 2020 confirms the aforementioned claim. The development of these technologies is driven by personal goals and international obligations in nations including the United States of America, China, India, Japan, South Korea, and several European nations. On the other hand, the efficiency of the fuel cell is affected by the quantum species (electron, proton, hydrogen and oxygen) formed during the interaction of inlet fuel (hydrogen and oxygen) with platinum. KN cross section during the collision of free electrons with atoms (H-atom and Pt-atom) close to the cathode of proton exchange membrane fuel cells (PEMFCs) is the goal of this work. During the collision of free electrons with H and Pt atoms, respectively, the maximum KN cross section measured for single scattering is approximately 70.2 m^2 and 66.0 m^2. The maximum KN cross section recorded for 1ml flow of hydrogen is about -26.6 m^2 and -22.3 m^2 [12]. In 2004, Roy and Pratt used X-ray generator to test KN cross section theory with observations (from 11 to 40 keV) of the entire atom and the observations shows conventional sources ranged from 5% to 50%, but the measurements made with a synchrotron source indicated a small percentage difference. The Compton scattering measures in a range below 10 keV with a broader range of works using angles other than 90 and distinct atomic number Z values in order to confirm the sufficiency of the theoretical treatment.

The KN cross section behavior for H and Pt atoms is the main topic of the current investigation. Future studies may look into a larger range of topics to develop a more thorough grasp of the elements affecting the KN cross section. Understanding how these variables affect the KN cross section would require research into many elements with various atomic sizes, atomic numbers, and material characteristics. Dhobi et al. conducted research on the KN cross section for non-relativistic scenarios and the scattering zone surrounding the electrode in 2023. Furthermore, Dhobi et al. (2022) did not analyze the KN cross section in either the relativistic or non-relativistic case, but rather the interaction of quantum species created around the electrode of PEMFC [13]. There are numerous projects underway to increase the PEMFCs cell's efficiency through experimentation, theory, modeling, etc. Additionally, study is being done on scattering fields theoretically, practically, virtually, etc. However, there aren't many PEMFC and scattering coupled works. Given that PEMFC and scattered are both novel in the fields of research, academia, and industry. Consequently, it is crucial to research dispersion around the PEMFC electrode.

III. Methods and Materials

Hydrogen fuel cell electric vehicles (FCEVs), when compared with traditional internal combustion engine vehicles, they are more efficient from a different perspective. They have a range for driving of more than 300 miles and can be fueled similarly to vehicles with traditional internal combustion engines in around 5 minutes. The technology of FCEVs boost efficiency, like regenerative brakes that collect the electrical power lost during brakes and store it in batteries [14]. Due to their ease of use, quiet operation, high efficiency, and modular design, fuel cells (FCs) have attracted a lot of attention in the automotive sector in recent decades. The usage of FCs in electric automobiles (EVs) is predicted to grow quickly, spark a revolution, and eventually replace conventional vehicles, according to technological breakthroughs. Commercial cars, programs, and research demonstrate that efforts are being made to guarantee that FCEVs have performance improvements sufficient for daily transportation requirements. First, the application areas, distinguishing characteristics, and operational circumstances of FC types and electrical motors are reviewed. According to their structure, complexity, and architectural frequency of use, power converters—voltage regulating and motor drive topologies—that are employed in FCEVs are described in depth [15].

Free electrons, protons, and leftover hydrogen are created when hydrogen comes into touch with the electrodes' catalyst. When the formation electron collides with the atom of hydrogen, a great deal of collisions occurs in the system, which causes heat to be produced. However, in this instance, we take into account the collision that occurs of the hydrogen atom and a free electron. PEMFCs have a serious issue with fuel cell efficiency because of the heat produced during collisions. We are interested in studying the Kelin-Gordan differential cross section that results from the collision of an electron and a hydrogen atom. The classical Thomson scattering can be described using a generalized Klein-Nishina differential equation for Compton scattering with a limited train of pulses. The quantity of scattering photons produced at a particular solid angle $d\Omega$ is

$$\frac{dN_{scat}}{d\Omega} = \int_{-\infty}^{\infty} \frac{\epsilon_0 c|E_x(\omega)|^2}{2\pi\hbar|\omega|} \frac{d\sigma}{d\Omega} d\omega \qquad (3)$$

And because the scattered photon has energy $\hbar\omega'$, the total scattered energy is:

$$\frac{dU_r}{d\Omega} = \int_{\infty}^{\infty} \frac{\epsilon_0 c|E_x(\omega)|^2}{2\pi} \frac{\omega'}{\omega} \frac{d\sigma}{d\Omega} d\omega \qquad (4)$$

The input gamma ray impacts an atomic electron, causing atomic ionization, and this is the primary scattering mechanism that produces 511 Kev photons. The KN differential cross section formula will determine the angle at which the incident photon will scatter,

$$\left(\frac{d\sigma}{d\Omega}\right)_a = \frac{Zr_e^2}{2}\left(\frac{1}{1+\alpha(1-cos\theta)}\right)^2 \left((1+\cos^2\theta) + \frac{\alpha^2(1-cos\theta)^2}{[1+\alpha(1-cos\theta)]}\right) \qquad (5)$$

A variation of the differential atomic cross sectional area equations for K-N can be found here. Additionally, Knoll discovered the complete KN cross section per atom in 1989;

$$\sigma_a = 2\pi \int_0^{\pi} \left(\frac{d\sigma}{d\Omega}\right)_a sin\theta d\theta \qquad (6)$$

Where θ is scattering angle overall photons. Now from (5) and (6), we get:

$$\sigma_a = 2\pi \int_0^{\pi} \frac{Zr_e^2}{2}\left(\frac{1}{1+\alpha(1-cos\theta)}\right)^2 \left((1+\cos^2\theta) + \frac{\alpha^2(1-cos\theta)^2}{[1+\alpha(1-cos\theta)]}\right) sin\theta d\theta \tag{7}$$

After solving, the following is the total KN cross section per atom:

$$\sigma_a = Z2\pi r_e^2 \left\{\frac{1+\alpha}{\alpha^2}\left[\frac{2(1+\alpha)}{1+2\alpha} - \frac{\ln(1+2\alpha)}{\alpha}\right] + \frac{\ln(1+2\alpha)}{2\alpha} - \frac{1+3\alpha}{(1+2\alpha)^2}\right\} \tag{8}$$

Since electronic cross-sections are multiplied by each element's charge number Z to get Klein-Nishina atomic cross-sections, equation (7) states that $\sigma_a = Z.\sigma_e$ the electronic cross-sectional area for KN is

$$\sigma_e = 2\pi r_e^2 \left\{\frac{1+\alpha}{\alpha^2}\left[\frac{2(1+\alpha)}{1+2\alpha} - \frac{\ln(1+2\alpha)}{\alpha}\right] + \frac{\ln(1+2\alpha)}{2\alpha} - \frac{1+3\alpha}{(1+2\alpha)^2}\right\} \tag{9}$$

where $r_e = 2.818\, fm$ is the classical electron radius, Z is the nuclear charge of the target molecule and $\alpha = \frac{E}{m_e c^2} = \frac{E}{0.511MeV}$, for non relativistic case. For relativistic case, energy of electron $E_r = \frac{mc^2}{\sqrt{1-v^2/c^2}} = \frac{mc^2}{\sqrt{\beta}}$ [16] and $mc^2 = 0.511MeV$ [17]. Also, $E_r = \frac{1}{\sqrt{1-v^2/c^2}}$ therefore for relativistic case $\alpha_r = \frac{1}{\sqrt{1-v^2/c^2}}$. Now equation (11) can be modified as

$$\sigma_e^r = 2\pi r_e^2 \left\{\frac{1+\alpha_r}{\alpha_r^2}\left[\frac{2(1+\alpha_r)}{1+2\alpha_r} - \frac{\ln(1+2\alpha_r)}{\alpha_r}\right] + \frac{\ln(1+2\alpha_r)}{2\alpha_r} - \frac{1+3\alpha_r}{(1+2\alpha_r)^2}\right\} \tag{10}$$

Also from, $\sigma_a = Z.\sigma_e$ we have

$$\sigma_a^r = 2Z\pi r_e^2 \left\{\frac{1+\alpha_r}{\alpha_r^2}\left[\frac{2(1+\alpha_r)}{1+2\alpha_r} - \frac{\ln(1+2\alpha_r)}{\alpha_r}\right] + \frac{\ln(1+2\alpha_r)}{2\alpha_r} - \frac{1+3\alpha_r}{(1+2\alpha_r)^2}\right\} \tag{11}$$

IV. Results and Discussion

The KN cross sections for electron and atom interactions are shown in Figure 1 as a function of electron energy. With increased electron energy, the cross section is seen to decrease. The cross section is initially large at lower energy, indicating a greater likelihood of interaction. But as electron energy rises, the cross section gradually contracts until it reaches a fixed value. It is clear from comparing the cross sections of platinum and hydrogen that platinum has a higher KN cross section than hydrogen and electronic interaction. The size of the atoms under consideration accounts for the majority of this variation.

Platinum atoms' increased size increases the scattering likelihood and raises the cross section.

By taking into account the energy dependency of scattering processes, it is possible to explain the decreasing pattern of the KN cross section with rising electron energy. Because their energy scales are more closely matched at lower energies, the relationship between an incoming electron and the object being targeted atom has a greater impact. The contact, however, weakens with increasing electron energy, resulting in a decrease in the width of the cross section. The significance of atomic size is demonstrated by comparing the cross sections of hydrogen and platinum. The cross section of platinum is higher because platinum atoms are bigger than hydrogen atoms. This is explained by the fact that there are more scattering centers accessible, which increases the likelihood of scattering occurrences. The KN cross section obtains a constant value in the high-energy area. This tendency implies that the incident electron's interaction with the target atom weakens and becomes less reliant on electron energy. Due to the predominance of relativistic effects, whereby the wavelength of the input electron shrinks dramatically relative to the size of the scattering centers, the interaction is diminished.

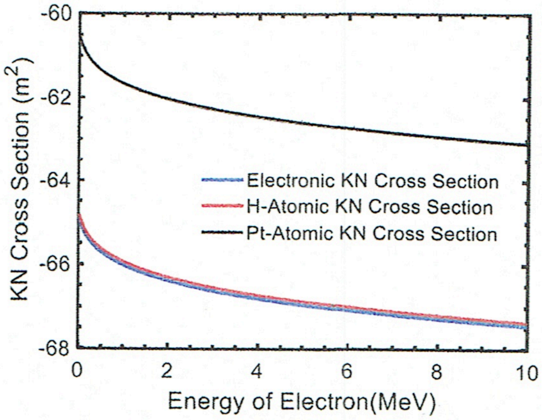

Figure 1: KN cross section with electron energy

Figures 2, 3, and 4 depict the KN electron and atomic cross section together with the electron's velocity. The KN electronic and atomic cross sections fall exponentially with increasing energy of electrons in the relativistic situation. The two main causes of this phenomena are the contraction of the electron wavelength and the relativistic mass increase. For the relativistic situation of mass, an electron's mass grows noticeably when it approaches relativistic energies, which are energy close to the speed of light. The relativistic mass of an object traveling at a high speed is determined by, in accordance with Einstein's theory of special relativity. The trajectory of the electrons during scattering events is impacted by the increase in mass. At greater energies, the electron behaves resembles a heavy particle because its relativistic mass is much more than its rest mass. The KN cross section decreases as a result of the higher mass since it lowers the likelihood of scattering.

In the relativistic wavelength situation, the electron's wavelength gets shorter as its energy rises. An electron's de Broglie wavelength is calculated using the formula ($\lambda = h/p$), where λ is the wavelength, h is Planck's constant, and p is the electron's momentum. A shortened de Broglie wavelength results from the electron's momentum increasing as its energy does. By decreasing the true dimension of the scattered centers (atoms), the diminishing electron wavelength has an impact on the scattering process. The efficiency of scattering decreases when the wavelength of the electron approaches or falls below the dimensions of the scattering centers. The KN cross section decreases as a result of this decline in scattering effectiveness. As a result, the KN electronic and atomic cross sections exponentially drop with increasing electron energy due to the interaction between the relativistic mass increase and the decreasing electron wavelength in the relativistic regime.

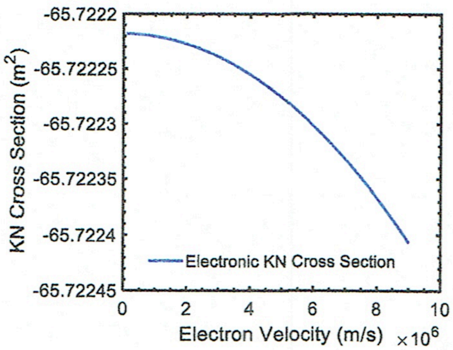

Figure 2: KN Electronic cross section with electron energy

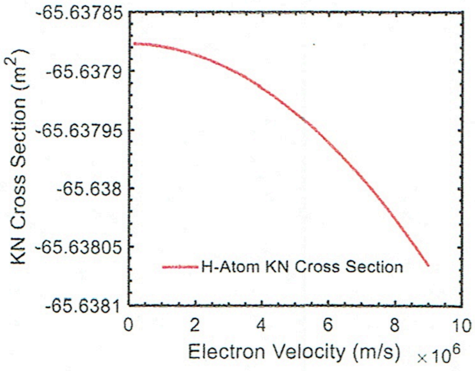

Figure 3: H-Atom KN cross section with electron energy

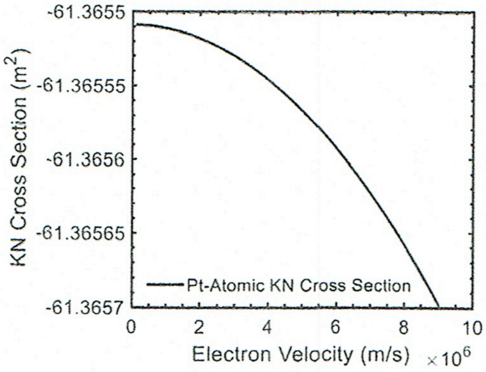

Figure 4: Pt-Atom KN cross section with electron energy

The KN cross section for Pt is greater than the KN cross section for hydrogen (H), as well as the KN electronic cross section, when the KN cross sections from Figures 2, 3, and 4 are compared. Additionally, it is discovered that the KN cross section for hydrogen is greater than that of the KN electronic cross section. There are various underlying causes for this variation in cross section values. The atomic size of the particles that interact is a significant factor for the observed variations in the KN cross sections. Hydrogen atoms are much smaller than platinum atoms. Due to their bigger size, platinum atoms offer a larger target region for the incoming electrons to engage with during the scattering process. Since there are more scattering events as a result, platinum has a greater cross section than hydrogen and electronic interactions.

The target atoms' atomic number is another element that affects the cross section discrepancy. Compared to hydrogen, Pt has a higher atomic number. Higher atomic numbers equate to more electrons in the atom's outer shells, which increases the number of potential places for interaction for the incoming electrons and affects the scattering likelihood. As a result, platinum has a greater cross section than electrical and hydrogen interactions. The difference in cross section between electronic interactions and hydrogen is also influenced by the electron binding effects. The attractive force of the charged proton in its nucleus is felt by an incident electron when it comes into contact with a hydrogen atom. In comparison to the KN electronic cross section, which solely takes into account the scattering of electrons without taking into account the influence of a bonded nucleus, this attractive force increases the scatter probability, resulting in a greater KN cross section for hydrogen.

Overall, the differences in the KN cross sections are caused by the interaction of atomic size, atomic number, and electron binding effects. Platinum has a bigger cross section than hydrogen and electrical interactions due to its bigger dimensions and higher atomic number. In addition, compared to electronic interactions, the effects of hydrogen's electron binding contribute to its greater cross section.

It is found that the KN cross section in the relativistic case is greater than in the non-relativistic case when compared the KN cross sections in the relativistic and non-relativistic instances, as shown in figure 5. The scattering is governed by classical electromagnetic theory in the non-relativistic situation, where the electron energies are substantially lower than the speed of light (c). Assuming the amount of electron mass stays constant during the scattered process and ignoring relativistic effects, Thomson scattering is used to characterize the cross section for this case. On the other hand, relativistic effects become important in the case where the electron energy approach or surpass a large proportion of the speed of light. The KN formula, which integrates relativistic adjustments to the scatter amplitude and accounts for the fluctuation of electrons mass with energy, describes relativistic scattering.

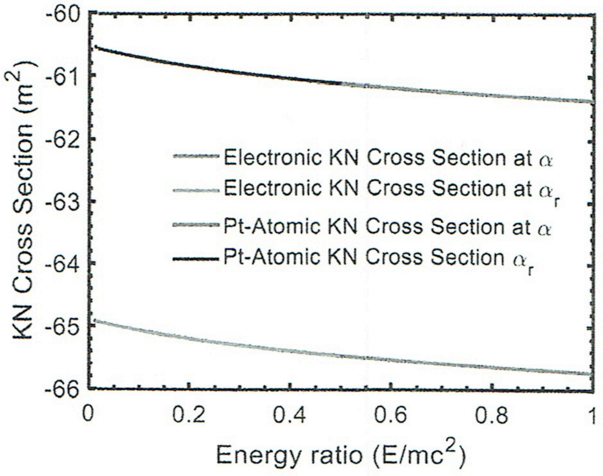

Figure 5: KN cross section with energy ratio for relativistic and non-relativistic case

Additionally, the electron's mass greatly increases in the relativistic zone as its kinetic energy approach the speed of light. The enhanced contact between an incoming electron and the intended atom caused by the higher mass has an impact on the scattering process. A higher scatter probability and, as a result, a greater KN cross section are produced by this increased contact. The KN formula considers the energy dependency of the scattering process while calculating the relativistic scattering amplitude. When an electron is struck at a greater energy, its wavelength approaches or even falls below the dimension of the scattering centers (atoms). Comparing to the non-relativistic scenario, this enables more effective scattering and increases the cross section. As a result, the relativistic situation has a greater KN cross section than the non-relativistic case due to the combination of the relativistic mass increases and the dependent on energy scattering amplitude. The increased cross section is due to relativistic phenomena that increase the scattering probability and enable stronger interactions among the incoming electron and the target atom.

V. Conculsion

In conclusion, the energy dependency of scattering processes can be used to explain the declining tendency of the KN cross section increasing electron energy. In comparing the cross sections of hydrogen and platinum, it is clear how important atomic size and number are; platinum has a higher cross section because of its bigger dimensions and greater atomic number. Additionally, the KN cross section remains constant in the high-energy area, indicating weaker and fewer energy-dependent interactions, possibly as a result of relativistic processes. The KN cross section is found to be greater in the relativistic domain when compared the relativistic and non-relativistic situations. This is attributable to the relativistic mass rise and energy-dependent scattered amplitude. A larger range of atomic sizes, numbers, and substances should be investigated in order to better comprehend KN cross sections. Radiation therapy, medical imaging, and materials science can all benefit from the findings. Computer simulations are useful for understanding complex systems.

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